2,3-Dihydroxynaphthalene 92-44-4 | DTXSID2043903

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	1.14	0.85	1.12	0.83	1.23	

Model Results

Predicted value: 3.53e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.02e-01

Confidence level: 6.96e-01

Nearest Neighbors from the Training Set

Image not found

1,4-Benzoquinone Measured: 4.60e-12 Predicted: 5.97e-12

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2-Methyl-p-benzoquinone Measured: 2.35e-11 Predicted: 2.15e-11

Image not found

1,3,5-Cycloheptatriene Measured: 9.69e-11 Predicted: 1.00e-10